Streamlining the process of materials discovery

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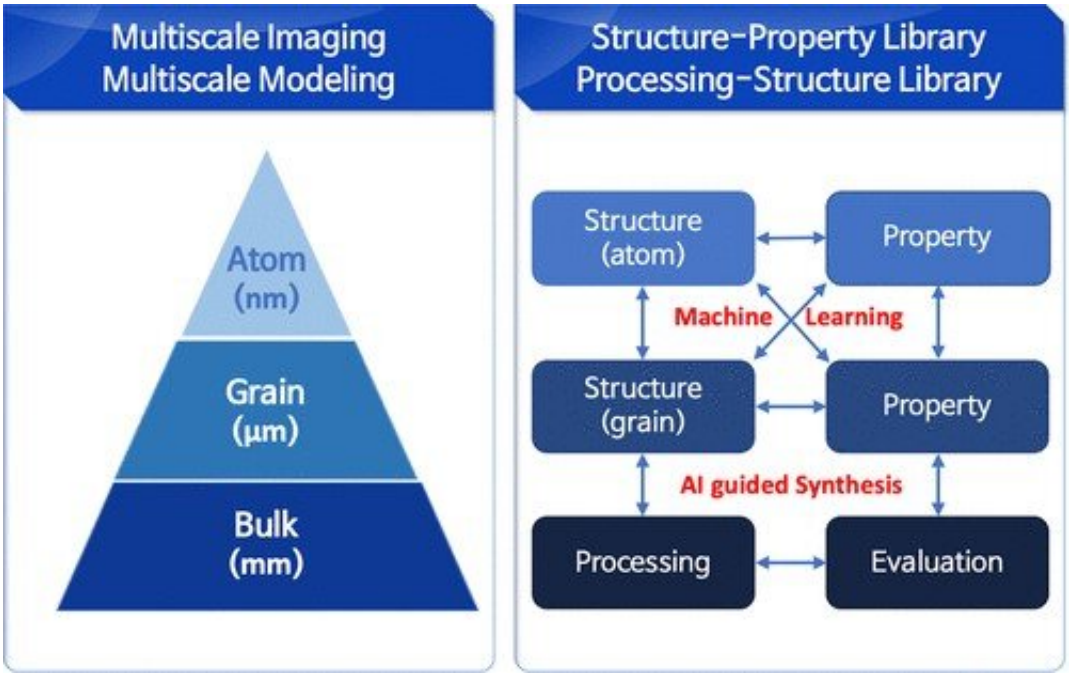

Figure 1. Schematic diagram of the M3I3 Flagship Project. This project aims to achieve the seamless integration of the multiscale "structure-property" and "processing-property" relationships via materials modeling, imaging, and machine learning. With the capability of artificial intelligence (AI)-guided automatic synthesis, M3I3 will provide expedited development of new materials in the near future. Credit: KAIST

Developing new materials and novel processes has continued to change the world. The M3I3 Initiative at KAIST has led to new insights into advancing materials development by implementing breakthroughs in

materials imaging that have created a paradigm shift in the discovery of materials. The Initiative features the multiscale modeling and imaging of structure and property relationships and materials hierarchies combined with the latest material-processing data.

The research team led by Professor Seungbum Hong analyzed the materials research projects reported by leading global institutes and research groups, and derived a quantitative model using machine learning with a scientific interpretation. This process embodies the research goal of the M3I3: Materials and Molecular Modeling, Imaging, Informatics and Integration.

The researchers discussed the role of multiscale materials and molecular imaging combined with machine learning and also presented a future outlook for developments and the major challenges of M3I3. By building this model, the research team envisions creating desired sets of properties for materials and obtaining the optimum processing recipes to synthesize them.

"The development of various microscopy and diffraction tools with the ability to map the structure, property, and performance of materials at multiscale levels and in real time enabled us to think that materials imaging could radically accelerate materials discovery and development," says Professor Hong.

"We plan to build an M3I3 repository of searchable structural and property maps using FAIR (Findable, Accessible, Interoperable, and Reusable) principles to standardize best practices as well as streamline the training of early career researchers."

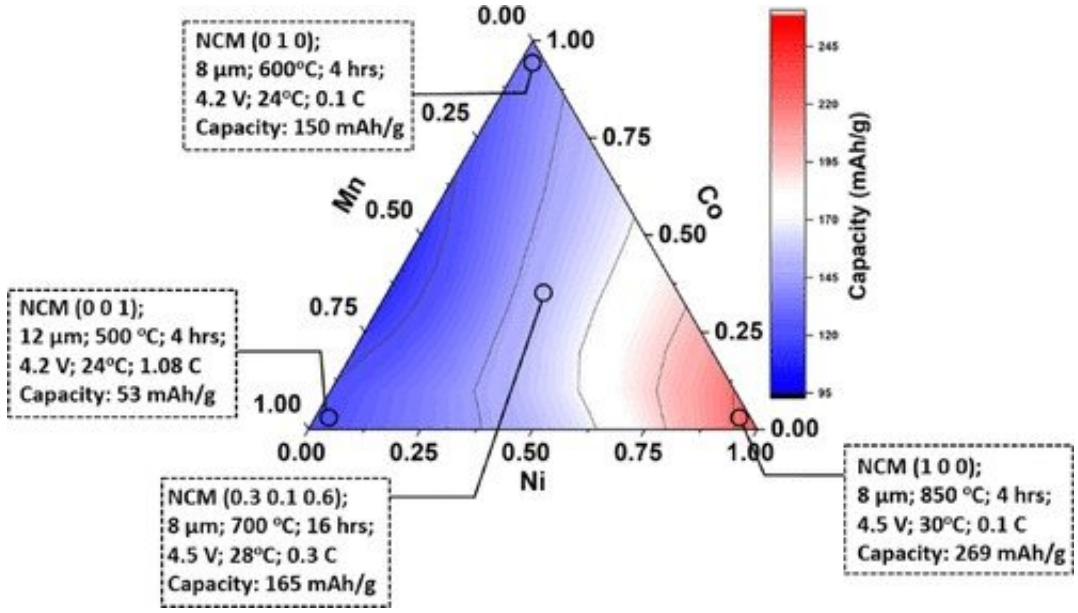

Figure 2. Capacity contour triangle plot as functions of composition (Ni, Co, and Mn), particle size, sintering temperature/time, measurement temperature, cutoff voltage, and C-rate. Credit: KAIST

One of the examples that shows the power of structure-property imaging at the nanoscale is the development of future materials for emerging nonvolatile memory devices. Specifically, the research team focused on microscopy using photons, electrons, and physical probes on the multiscale structural hierarchy, as well as structure-property relationships to enhance the performance of memory devices.

"M3I3 is an algorithm for performing the reverse engineering of future materials. Reverse engineering starts by analyzing the structure and composition of cutting-edge materials or products. Once the research team determines the performance of our targeted future materials, we need to know the candidate structures and compositions for producing the future materials."

The research team has built a data-driven experimental design based on

traditional NCM (nickel, cobalt, and manganese) cathode materials. With this, the research team expanded their future direction for achieving even higher discharge capacity, which can be realized via Li-rich cathodes.

However, one of the major challenges was the limitation of available data that describes the Li-rich cathode properties. To mitigate this problem, the researchers proposed two solutions: First, they should build a machine-learning-guided data generator for data augmentation. Second, they would use a machine-learning method based on 'transfer learning.' Since the NCM cathode database shares a common feature with a Li-rich cathode, one could consider repurposing the NCM trained model for assisting the Li-rich prediction. With the pretrained model and transfer learning, the team expects to achieve outstanding predictions for Li-rich cathodes even with the small data set.

With advances in experimental imaging and the availability of well-resolved information and big data, along with significant advances in high-performance computing and a worldwide thrust toward a general, collaborative, integrative, and on-demand research platform, there is a clear confluence in the required capabilities of advancing the M3I3 Initiative.

Professor Hong said, "Once we succeed in using the inverse "property-structure-processing" solver to develop cathode, anode, electrolyte, and membrane materials for high energy density Li-ion batteries, we will expand our scope of materials to battery/fuel cells, aerospace, automobiles, food, medicine, and cosmetic materials."

More information: Seungbum Hong et al, Reducing Time to Discovery: Materials and Molecular Modeling, Imaging, Informatics, and Integration, *ACS Nano* (2021). DOI: 10.1021/acsnano.1c00211

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